

=> d his

(FILE 'HOME' ENTERED AT 03:49:07 ON 01 JUL 2002)

FILE 'REGISTRY' ENTERED AT 03:49:14 ON 01 JUL 2002

L1 STRUCTURE UPLOADED

L2 1 S L1

L3 79 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 03:49:50 ON 01 JUL 2002

L4 43 S L3

L5 25 S L4 AND PD < MAY 1998

L6 5 S L4 AND READ, R?/AU

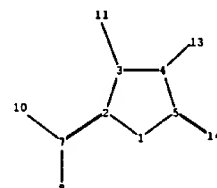
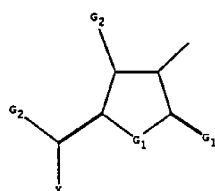
L7 24 S L5 NOT L6

FILE 'CAOLD' ENTERED AT 03:51:30 ON 01 JUL 2002

=> s 13

L8 0 L3

2023-9-5 13:34
Sally Terry



chain nodes :

7 8 10 11 13 14

ring nodes :

1 2 3 4 5

chain bonds :

2-7 3-11 4-13 5-14 7-8 7-10

ring bonds :

1-2 1-5 2-3 3-4 4-5

exact/norm bonds :

1-2 1-5 2-3 2-7 3-4 3-11 4-5 4-13 5-14 7-8 7-10

isolated ring systems :

containing 1 :

G1:O,S

G2:X,H

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:CLASS 8:CLASS 10:CLASS 11:CLASS 13:CLASS
14:Atom

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssspta1612BXR

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TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2	Jan 25	BLAST(R) searching in REGISTRY available in STN on the Web
NEWS 3	Jan 29	FSTA has been reloaded and moves to weekly updates
NEWS 4	Feb 01	DKILIT now produced by FIZ Karlsruhe and has a new update frequency
NEWS 5	Feb 19	Access via Tymnet and SprintNet Eliminated Effective 3/31/02
NEWS 6	Mar 08	Gene Names now available in BIOSIS
NEWS 7	Mar 22	TOXLIT no longer available
NEWS 8	Mar 22	TRCTHERMO no longer available
NEWS 9	Mar 28	US Provisional Priorities searched with P in CA/CAPLUS and USPATFULL
NEWS 10	Mar 28	LIPINSKI/CALC added for property searching in REGISTRY
NEWS 11	Apr 02	PAPERCHEM no longer available on STN. Use PAPERCHEM2 instead.
NEWS 12	Apr 08	"Ask CAS" for self-help around the clock
NEWS 13	Apr 09	BEILSTEIN: Reload and Implementation of a New Subject Area
NEWS 14	Apr 09	ZDB will be removed from STN
NEWS 15	Apr 19	US Patent Applications available in IFICDB, IFIPAT, and IFIUDB
NEWS 16	Apr 22	Records from IP.com available in CAPLUS, HCAPLUS, and ZCAPLUS
NEWS 17	Apr 22	BIOSIS Gene Names now available in TOXCENTER
NEWS 18	Apr 22	Federal Research in Progress (FEDRIP) now available
NEWS 19	Jun 03	New e-mail delivery for search results now available
NEWS 20	Jun 10	MEDLINE Reload
NEWS 21	Jun 10	PCTFULL has been reloaded
NEWS EXPRESS		February 1 CURRENT WINDOWS VERSION IS V6.0d, CURRENT MACINTOSH VERSION IS V6.0a(ENG) AND V6.0Ja(JP), AND CURRENT DISCOVER FILE IS DATED 05 FEBRUARY 2002
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FILE 'HOME' ENTERED AT 03:49:07 ON 01 JUL 2002

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 03:49:14 ON 01 JUL 2002
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STRUCTURE FILE UPDATES: 28 JUN 2002 HIGHEST RN 435268-39-6
DICTIONARY FILE UPDATES: 28 JUN 2002 HIGHEST RN 435268-39-6

TSCA INFORMATION NOW CURRENT THROUGH January 7, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

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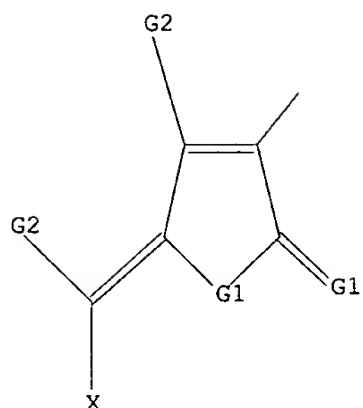
Uploading 09673305.str

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR



G1 O,S

G2 X,H

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 03:49:39 FILE 'REGISTRY'
 SAMPLE SCREEN SEARCH COMPLETED - 147 TO ITERATE

100.0% PROCESSED 147 ITERATIONS 1 ANSWERS
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
 PROJECTED ITERATIONS: 2213 TO 3667
 PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

=> s l1 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 139.90 U.S. DOLLARS
 DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 03:49:45 FILE 'REGISTRY'
 FULL SCREEN SEARCH COMPLETED - 3462 TO ITERATE

100.0% PROCESSED 3462 ITERATIONS 79 ANSWERS
 SEARCH TIME: 00.00.02

L3 79 SEA SSS FUL L1

=> file hcaplus

COST IN U.S. DOLLARS

SINCE FILE TOTAL
 ENTRY SESSION

FULL ESTIMATED COST 140.28 140.49

FILE 'HCAPLUS' ENTERED AT 03:49:50 ON 01 JUL 2002
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FILE COVERS 1907 - 1 Jul 2002 VOL 137 ISS 1
 FILE LAST UPDATED: 30 Jun 2002 (20020630/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

=> s 13

L4 43 L3

=> s 14 and pd < may 1998

18832374 PD < MAY 1998
 (PD<19980500)

L5 25 L4 AND PD < MAY 1998

=> s 14 and read, r?/au

394 READ, R?/AU
 L6 5 L4 AND READ, R?/AU

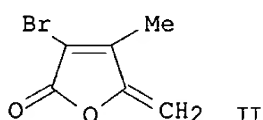
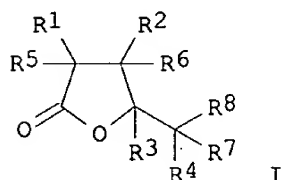
=> d 16, ibib abs fhitr, 1-5

L6 ANSWER 1 OF 5 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 2002:10458 HCAPLUS
 DOCUMENT NUMBER: 136:69697
 TITLE: Preparation and antimicrobial activity of fimbrolides
 INVENTOR(S): Kumar, Naresh; Read, Roger Wayne
 PATENT ASSIGNEE(S): Unisearch Limited, Australia
 SOURCE: PCT Int. Appl., 77 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent

LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002000639	A1	20020103	WO 2001-AU781	20010628
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
PRIORITY APPLN. INFO.:			AU 2000-8419	A 20000628
OTHER SOURCE(S):			CASREACT 136:69697; MARPAT 136:69697	

GI



AB Fimbrolides, such as I [R1 = H, halogen, alkyl; R2 = alkyl, alkoxy, oxoalkyl, alkenyl, aryl, arylalkyl; R3 = H, OH, halogen, alkoxy; R4, R8 = H, halogen; R7 = H; R5, R6 = H, halogen; R3R7 = bond; R5R6 = bond], were prepd. for use as antibacterial and fungicidal agents. Thus, furanone II was prepd. in a four step synthetic sequence, which included condensation of OHCCO2H with MeCOCH2Me to form MeCOC(Me):CHCO2H, bromination to form MeCOCBrMeCHBrCO2H, lactonization to form I (R1 = R2 = Br, R3R7 = bond, R4 = R5 = R8 = H, R6 = Me), and dehydrobromination as the final step. The prepd. furanones were tested for their ability to inhibit biofilm formation by *Pseudomonas aeruginosa* and for antibacterial and fungicidal activity against *Staphylococcus aureus* and *Candida albicans*.

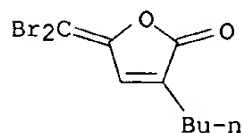
IT **174862-78-3P**

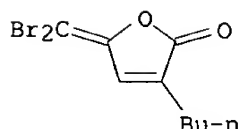
RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. and antimicrobial activity of fimbrolides)

RN 174862-78-3 HCAPLUS

CN 2(5H)-Furanone, 3-butyl-5-(dibromomethylene)- (9CI) (CA INDEX NAME)





REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L6 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2001:762818 HCAPLUS

DOCUMENT NUMBER: 135:308957

TITLE: Antimicrobial coatings containing furanones

INVENTOR(S): **Read, Roger**; Kumar, Naresh; Wilcox, Mark;
Zhu, Hua; Griesser, Hans; Muir, Ben; Thissen, Helmut;
Hughes, Tim

PATENT ASSIGNEE(S): Unisearch Limited, Australia

SOURCE: PCT Int. Appl., 27 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001076594	A1	20011018	WO 2001-AU407	20010410
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
PRIORITY APPLN. INFO.:			AU 2000-6812	A 20000410

OTHER SOURCE(S): MARPAT 135:308957

AB The present invention provides a substrate having a plurality of immobilized furanone moieties assocd. with at least part of a surface of the substrate. The substrate is selected from metals, ceramics, glasses, natural polymers, synthetic polymers, and natural materials, such as fibers, wool, hair, silk, cotton, collagen, etc. The invention also relates to articles consisting of or comprising such a substrate. For example, a furanone deriv. was immobilized onto amine poly(acrylic acid) and azidoaniline-coated polyfluorinated poly(ethylene-co-propylene) (Teflon FEP) showing a redn. of bacterial adhesion of 35% (initial adhesion) and 62% for biofilm formation.

IT **63025-21-8**

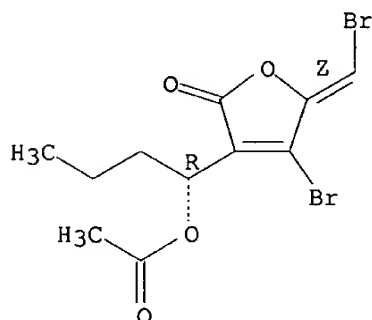
RL: RCT (Reactant); RACT (Reactant or reagent)

(furanones immobilization on biomaterials as antimicrobial coatings)

RN 63025-21-8 HCAPLUS

CN 2(5H)-Furanone, 3-[(1R)-1-(acetyloxy)butyl]-4-bromo-5-(bromomethylene)-, (5Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L6 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1999:691095 HCAPLUS

DOCUMENT NUMBER: 131:296526

TITLE: Preparation of fimbrolide analog fouling inhibitors
and bactericides

INVENTOR(S): **Read, Roger**; Kumar, Naresh

PATENT ASSIGNEE(S): Unisearch Limited, Australia

SOURCE: PCT Int. Appl., 52 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9954323	A1	19991028	WO 1999-AU285	19990416
W:	AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
CA 2328364	AA	19991028	CA 1999-2328364	19990416
AU 9933225	A1	19991108	AU 1999-33225	19990416
EP 1071677	A1	20010131	EP 1999-914366	19990416
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI			

PRIORITY APPLN. INFO.: AU 1998-2978 A 19980416

WO 1999-AU285 W 19990416

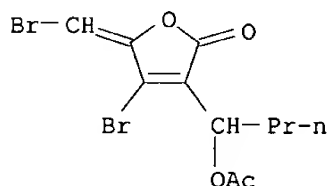
OTHER SOURCE(S): CASREACT 131:296526; MARPAT 131:296526

AB The invention relates to the side chain functionalization of fimbrolides (halogenated 3-alkyl-5-methylene-2(5H)-furanones) and their synthetic analogs, that yields fimbrolides substituted with a halogen, an oxygen or a nitrogen functionality in the alkyl chain, esp. fimbrolide alcs., carboxylate and sulfinic and sulfonic esters, ethers, aldehydes, ketones, acids, amides, nitro derivs., hydrophobic, hydrophilic and fluorophilic alkyl derivs. and polymers (Markush given). The fimbrolide analogs are bactericides and marine fouling inhibitors.

IT **169274-84-4P**
 RL: BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (prepn. as fimbrolide analog fouling inhibitor and bactericide)

RN 169274-84-4 HCAPLUS

CN 2(5H)-Furanone, 3-[1-(acetyloxy)butyl]-4-bromo-5-(bromomethylene)- (9CI)
 (CA INDEX NAME)



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L6 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1999:154230 HCAPLUS

DOCUMENT NUMBER: 130:348124

TITLE: Evidence that halogenated furanones from *Delisea pulchra* inhibit acylated homoserine lactone (AHL)-mediated gene expression by displacing the AHL signal from its receptor protein.

AUTHOR(S): Manefield, Michael; De Nys, Rocky; Kumar, Naresh; **Read, Roger**; Givskov, Michael; Steinberg, Peter; Kjelleberg, Staffan

CORPORATE SOURCE: School of Microbiology and Immunology, University of New South Wales, Sydney, Australia

SOURCE: Microbiology (Reading, United Kingdom) (1999), 145(2),

283-291

CODEN: MROBEO; ISSN: 1350-0872

PUBLISHER: Society for General Microbiology

DOCUMENT TYPE: Journal

LANGUAGE: English

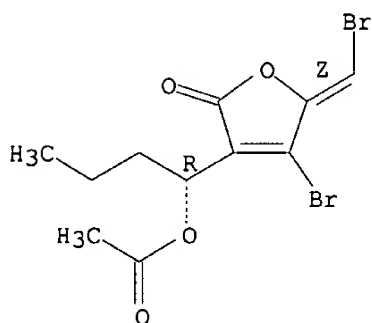
AB Acylated homoserine lactone (AHL)-mediated gene expression controls phenotypes involved in colonization, often specifically of higher organisms, in both marine and terrestrial environments. The marine red alga *Delisea pulchra* produces halogenated furanones which resemble AHLs structurally and show inhibitory activity at ecol. realistic concns. in AHL bioassays. Evidence is presented that halogenated furanones displace tritiated OHHL [N-3-(oxohexanoyl)-L-homoserine lactone] from *Escherichia*

coli cells overproducing LuxR with potencies corresponding to their resp. inhibitory activities in an AHL-regulated bioluminescence assay, indicating that this is the mechanism by which furanones inhibit AHL-dependent phenotypes. Alternative mechanisms for this phenomenon are also addressed. General metabolic disruption was assessed with two-dimensional PAGE, revealing limited non-AHL-related effects. A direct chem. interaction between the algal compds. and AHLs, as monitored by ¹H NMR spectroscopy, was shown not to occur in vitro. These results support the contention that furanones, at the concns. produced by the alga, can control bacterial colonization of surfaces by specifically interfering with AHL-mediated gene expression at the level of the LuxR protein.

IT 63025-21-8
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study) (evidence that halogenated furanones from *Delisea pulchra* inhibit acylated homoserine lactone (AHL)-mediated gene expression by displacing AHL signal from its receptor protein)

RN 63025-21-8 HCAPLUS
 CN 2(5H)-Furanone, 3-[(1R)-1-(acetyloxy)butyl]-4-bromo-5-(bromomethylene)-, (5Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry as shown.



REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L6 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1997:745270 HCAPLUS
 DOCUMENT NUMBER: 128:34643
 TITLE: Reinvestigation of the sulfuric acid-catalyzed cyclization of brominated 2-alkyllevulinic acids to 3-alkyl-5-methylene-2(5H)-furanones
 AUTHOR(S): Manny, Anthony J.; Kjelleberg, Staffan; Kumar, Naresh;
 de Nys, Rocky; Read, Roger W.; Steinberg, Peter
 CORPORATE SOURCE: Sch. Chem., Sch. Microbiol. Immunol., Sch. Biol. Sci.,

SOURCE: Univ. New South Wales, Sydney, NSW 2052, Australia
 Tetrahedron (1997), 53(46), 15813-15826
 CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

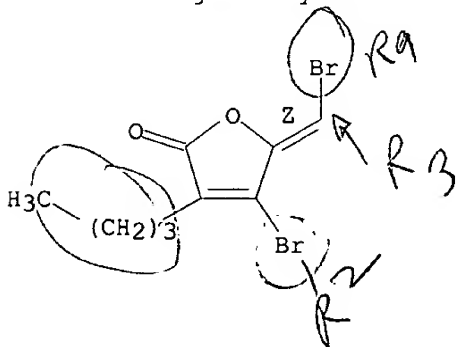
AB A synthesis of ethyl-, butyl-, hexyl- and dodecyl-substituted fimbrolide derivs. from (alkyl)levulinic acid derivs. through bromination and acid promoted lactonization was described. The underlying reactions were investigated using levulinic acid as a model, and the effects of varying the bromination conditions and changing acid concn. on product distribution are discussed. Dibromination proceeded best in CHCl₃ and proceeded in EtOH-free CHCl₃ without the complication of ester formation. Cyclization occurs with concomitant oxidn. in 98-100% H₂SO₄ but gave highest yields of fimbrolide derivs. in 100% H₂SO₄. The formation of related beckerelide substances is also described.

IT **63025-35-4P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (fimbrolide; prepn. of alkyl(methylene)furanones via lactonization of bromo(alkyl)levulinate derivs.)

RN 63025-35-4 HCAPLUS

CN 2(5H)-Furanone, 4-bromo-5-(bromomethylene)-3-butyl-, (5Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



=> d his

(FILE 'HOME' ENTERED AT 03:49:07 ON 01 JUL 2002)

FILE 'REGISTRY' ENTERED AT 03:49:14 ON 01 JUL 2002

L1 STRUCTURE UPLOADED
 L2 1 S L1
 L3 79 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 03:49:50 ON 01 JUL 2002

L4 43 S L3
 L5 25 S L4 AND PD < MAY 1998
 L6 5 S L4 AND READ, R?/AU

=> s 15 not 16

L7 24 L5 NOT L6

=> d 17, ibib abs fhitr, 1-24

L7 ANSWER 1 OF 24 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1998:178623 HCAPLUS

DOCUMENT NUMBER: 128:241398

TITLE: A new method for determining surface concentrations of

marine natural products on seaweeds

AUTHOR(S): De Nys, R.; Dworjanyn, S. A.; Steinberg, P. D.

CORPORATE SOURCE: School Biological Science, University New South Wales,

Sydney, 2052, Australia

SOURCE: Marine Ecology: Progress Series (1998), 162, 79-87

CODEN: MESEDT; ISSN: 0171-8630

PUBLISHER: Inter-Research

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A new technique is described for detg. the concn. of natural products on the surface of marine algae. Surface metabolites were quantified for 2 red algae, *Delisea pulchra* and *Laurencia obtusa*, by dipping the algae in hexane for 20-40 s at room temp. More stringent extn. procedures using other solvents or longer extn. times in hexane (>50 s) caused cell damage.

Natural products in the surface exts. were measured using GS/MS. Mean total surface concn. of natural products from *D. pulchra* were 250 ng/cm², but <1 ng/cm² for *L. obtusa*. These results contrast to whole plant levels

of total secondary metabolites in the 2 algae, which were higher in *L. obtusa* (7 .mu.g/mg dry wt.) than in *D. pulchra* (3.4 .mu.g/mg). Dipping thalli in hexane for 30 s also caused no cell lysis in 8 other species of macroalgae. It is suggested that the procedure is more broadly

applicable

for the quantification of non-polar surface metabolites on seaweeds and other organisms with resistant surface cells.

IT 63025-21-8

RL: ANT (Analyte); BOC (Biological occurrence); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study); OCCU (Occurrence)

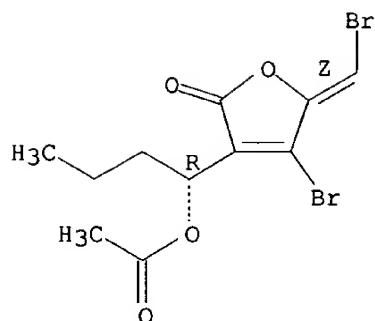
(method for detg. surface concns. of marine natural products on seaweeds)

RN 63025-21-8 HCAPLUS

CN 2(5H)-Furanone, 3-[(1R)-1-(acetyloxy)butyl]-4-bromo-5-(bromomethylene)-, (5Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



L7 ANSWER 2 OF 24 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1998:54252 HCAPLUS

DOCUMENT NUMBER: 128:177944

TITLE: Extracellular signal molecule(s) involved in the carbon starvation response of marine *Vibrio* sp.

strain

S14

AUTHOR(S): Srinivasan, Sujatha; Ostling, Jorgen; Charlton, Timothy; De Nys, Rocky; Takayama, Kathy; Kjelleberg, Staffan

CORPORATE SOURCE: School of Microbiology and Immunology, University of New South Wales, Sydney, 2052, Australia

SOURCE: Journal of Bacteriology (1998), 180(2), 201-209

CODEN: JOBAAY; ISSN: 0021-9193

PUBLISHER: American Society for Microbiology

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The role of exogenous metabolites as putative signal mols. mediating and/or regulating the carbon starvation adaptation program in *Vibrio* sp. strain S14 was investigated. Addn. of the stationary-phase supernatant ext. (SSE) of *Vibrio* sp. strain S14 to logarithmic-phase cells resulted

in

a significant no. of carbon starvation-induced proteins being up-regulated. Halogenated furanones, putative antagonists of acylated homoserine lactones (AHLs), inhibited the synthesis of proteins specifically induced upon carbon starvation. The effect of the furanone was the opposite of that caused by SSE with respect to the up- and down-regulation of protein expression, indicating that both the furanone and the putative signalling mols. were acting on the same regulatory pathway. Culturability was rapidly lost when *Vibrio* sp. strain S14 was starved in the presence of the furanone at a low concn. The furanone

also

had a neg. effect on the ability of carbon-starved cells to mount resistance against UV irradiation and hydrogen peroxide exposure. The SSE of *Vibrio* sp. strain S14 had the ability to provide cross-protection against the loss in viability caused by the furanone. We have further demonstrated that the SSE taken from low- as well as high-cell-d.

cultures

of *Vibrio* sp. strain S14 induced luminescence in *Vibrio harveyi*. Taken together, the results in this report provide evidence that *Vibrio* sp.

strain S14 produces extracellular signalling metabolites during carbon and energy starvation and that these mols. play an important role in the expression of proteins crucial to the development of starvation- and stress-resistant phenotypes.

IT 63025-35-4

RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); BUU (Biological use, unclassified); BIOL (Biological

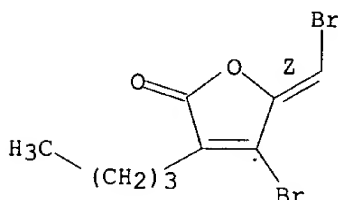
study); USES (Uses)

(inhibitor; extracellular signal mol.(s) involved in the carbon starvation response of marine *Vibrio* S14)

RN 63025-35-4 HCAPLUS

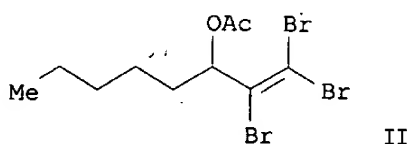
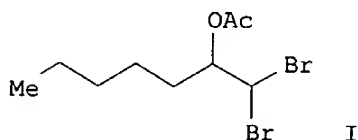
CN 2(5H)-Furanone, 4-bromo-5-(bromomethylene)-3-butyl-, (5Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L7 ANSWER 3 OF 24 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1997:164893 HCAPLUS
 DOCUMENT NUMBER: 126:141818
 TITLE: New Acetyl Derivatives from Antarctic *Delisea fimbriata*
 AUTHOR(S): Cueto, Mercedes; Darias, Jose; San-Martin, Aurelio; Rovirosa, Juana
 CORPORATE SOURCE: Instituto de Productos Naturales y Agrobiologia de Canarias, CSIC. Avda. Astrofisico Fco. Sanchez 3, La Laguna, 38206, Spain
 SOURCE: Journal of Natural Products (1997), 60(3), 279-281
 CODEN: JNPRDF; ISSN: 0163-3864
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI

QH1.L94



AB Compds. with three characteristic skeletons of members of the family Bonnemaisoneaceae were found to coexist in the alga *Delisea fimbriata*. The two new acetates I and II were also isolated; this is the first isolation of acetates from this genus. The structures, chem. transformation, and biogenetic significance of I and II are described.

IT 63025-34-3

RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(from Antarctic *Delisea fimbriata*)

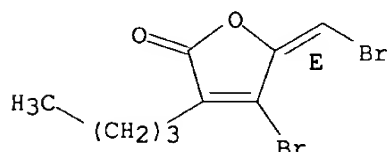
RN 63025-34-3 HCAPLUS

CN 2(5H)-Furanone, 4-bromo-5-(bromomethylene)-3-butyl-, (E)- (9CI) (CA

INDEX

NAME)

Double bond geometry as shown.



L7 ANSWER 4 OF 24 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1996:731975 HCAPLUS

DOCUMENT NUMBER: 126:4540

TITLE: Methods for microbial regulation

INVENTOR(S): Kjelleberg, Staffan; Steinberg, Peter; De, Nys Peter
Canisius; Maximilien, Ria; Manefield, Michael;
Givskov, Michael; Gram, Lone

PATENT ASSIGNEE(S): Unisearch Limited, Australia

SOURCE: PCT Int. Appl., 29 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

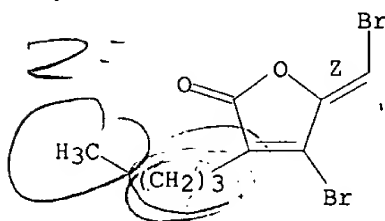
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9629392	A1	19960926	WO 1996-AU167	19960325 <--
W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN				
CA 2215797	AA	19960926	CA 1996-2215797	19960325 <--
AU 9649996	A1	19961008	AU 1996-49996	19960325 <--
AU 708962	B2	19990819		
EP 815201	A1	19980107	EP 1996-906677	19960325 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				

BR 9607661 A 19980616 BR 1996-7661 19960325
 CN 1185173 A 19980617 CN 1996-194117 19960325
 JP 11502108 T2 19990223 JP 1996-527912 19960325
 US 2002037578 A1 20020328 US 1998-913762 19980304
 PRIORITY APPLN. INFO.: AU 1995-1912 A 19950323
 WO 1996-AU167 W 19960325
 AB A method and microbial culture medium for inhibiting homoserine lactone-
 and/or acylated homoserine lactone-regulated processes in microorganisms
 using furanone compds. derived from *Delisea pulchra* or their chem.
 derivs.
 are claimed.
 IT 63025-35-4
 RL: BAC (Biological activity or effector, except adverse); BSU
 (Biological
 study, unclassified); BIOL (Biological study)
 (homoserine lactone- and/or acylated homoserine lactone-regulated
 processes in microorganisms inhibition by furanone derivs.)
 RN 63025-35-4 HCAPLUS
 CN 2(5H)-Furanone, 4-bromo-5-(bromomethylene)-3-butyl-, (5Z)- (9CI) (CA
 INDEX NAME)

Double bond geometry as shown.



L7 ANSWER 5 OF 24 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1996:666226 HCAPLUS
 DOCUMENT NUMBER: 125:296978
 TITLE: Inhibitory effects of secondary metabolites from the
 red alga *Delisea pulchra* on swarming motility of
Proteus mirabilis
 AUTHOR(S): Gram, Lone; De Nys, Rocky; Maximilien, Ria; Givskov,
 Michael; Steinberg, Peter; Kjelleberg, Staffan
 CORPORATE SOURCE: Sch. Microbiology and Immunology, Sch. Biolog. Sci.,
 Univ. New South Wales, Australia
 SOURCE: Appl. Environ. Microbiol. (1996), 62(11),
 4284-4287
 CODEN: AEMIDF; ISSN: 0099-2240
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Abnormal, uncoordinated swarming motility of the opportunistic human
 pathogen *Proteus mirabilis* was seen when a crude ext. of the Australian
 red alga *D. pulchra* was added to the medium. This occurred at concns. at
 which growth rate, swimming motility, cell elongation, polynucleation,
 and
 hyperflagellation were not affected. One halogenated furanone from *D.*
pulchra inhibited swarming motility at concns. that did not affect growth

rate and swimming motility. Other structurally similar *D. pulchra* furanones had no effect on swarming, suggesting considerable specificity in the effects of furanones on swarming motility by *P. mirabilis*.

IT 63025-27-4

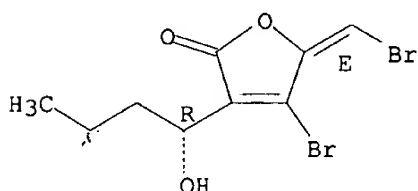
RL: BAC (Biological activity or effector, except adverse); BIOL (Biological study)

(inhibitory effect of furanone from red alga *Delisea pulchra* on swarming motility of *Proteus mirabilis*)

RN 63025-27-4 HCAPLUS

CN 2(5H)-Furanone, 4-bromo-5-(bromomethylene)-3-(1-hydroxybutyl)-, [R-(E)]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L7 ANSWER 6 OF 24 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1996:224398 HCAPLUS

DOCUMENT NUMBER: 124:284644

TITLE: Quantitative variation of secondary metabolites in the

sea hare *Aplysia parvula* and its host plant, *Delisea pulchra*

AUTHOR(S): Nys, Rocky de; Steinberg, Peter D.; Rogers, Cary N.; Charlton, Timothy S.; Duncan, Mark W.

CORPORATE SOURCE: School Biological Science, University New South Wales,

Sydney, 2052, Australia

SOURCE: Mar. Ecol.: Prog. Ser. (1996), 130(1 to 3), 135-46

CODEN: MESEDT; ISSN: 0171-8630

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The authors measured quant. variation of structurally similar halogenated furanones in the sea hare *Aplysia parvula* (Opisthobranchia; Anaspidea) and

in its host alga *Delisea pulchra* (Rhodophyta; Bonnemaisoniales). Mean total levels of furanones from *D. pulchra* in *A. parvula* were 13.3% of the dry wt. of the sea hares, with one metabolite comprising on av. 86% of the

total metabolite load of the sea hares. Levels of furanones in the sea hares were highest in the digestive gland but were also found in other tissues, including the skin in at least mg g⁻¹ (dry wt.) levels. Metabolite levels in the skin of the sea hares did not differ from those in *D. pulchra* (typically between 5 and 10 mg g⁻¹ dry wt.). Variation of metabolites in *D. pulchra* on the scale of both meters and kilometers was low and only minor variation in levels of individual metabolites was

obsd.

There was significant variation in levels of metabolites within plants, with concns. generally higher at the distal end of the thallus. The large differences in metabolite concns. on a scale of mm found in some other red algae were not obsd. in *D. pulchra*. Metabolites occurred in significantly different relative amts. in *A. parvula* vs. *D. pulchra*, with concns. of individual metabolites in *A. parvula* ranging between 0 and 83 times the concns. found in host algae. These results show that the sea hares differentially bioaccumulate algal metabolites. However, only 1 metabolite was enhanced in concn. in the sea hares relative to the alga. This metabolite was the most abundant compd. in the animals, and has been previously shown to be effective as a predator deterrent. A second metabolite, which was not effective as a predator deterrent in *A. parvula*, decreased in relative concn. in the animals. In contrast to recent suggestions in the literature for sequestered algal metabolites in sea hares, the results indicate that the distribution and level of *D. pulchra* metabolites in *A. parvula* are consistent with a role as acquired chem. defenses against predators.

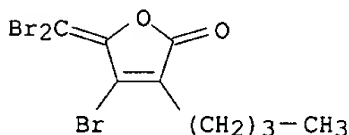
IT 63025-36-5

RL: BOC (Biological occurrence); BIOL (Biological study); OCCU (Occurrence)

(variation of halogenated furanone secondary metabolites in sea hare and its host plant, *Delisea pulchra*)

RN 63025-36-5 HCAPLUS

CN 2(5H)-Furanone, 4-bromo-3-butyl-5-(dibromomethylene)- (9CI) (CA INDEX NAME)



L7 ANSWER 7 OF 24 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1996:196774 HCAPLUS

DOCUMENT NUMBER: 124:234956

TITLE: Antifouling marine compositions of furanone compounds

INVENTOR(S): Steinberg, Peter David; De Nys, Peter Canisius

PATENT ASSIGNEE(S): Unisearch Ltd., Australia

SOURCE: PCT Int. Appl., 32 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9601294	A1	19960118	WO 1995-AU407	19950705 <--
W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI,				

GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD,
 MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ,
 TM, TT
 RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT,
 LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE,
 SN, TD, TG

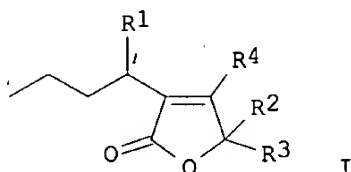
CA 2192955	AA	19960118	CA 1995-2192955	19950705 <--
AU 9528750	A1	19960125	AU 1995-28750	19950705 <--
AU 688535	B2	19980312		
EP 769039	A1	19970423	EP 1995-924107	19950705 <--
EP 769039	B1	20000927		

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT,
 SE

CN 1156471	A	19970806	CN 1995-194788	19950705 <--
CN 1047785	B	19991229		
JP 10502402	T2	19980303	JP 1995-503579	19950705 <--
AT 196643	E	20001015	AT 1995-924107	19950705
ES 2151962	T3	20010116	ES 1995-924107	19950705
US 6060046	A	20000509	US 1997-765226	19970218

PRIORITY APPLN. INFO.: AU 1994-6666 A 19940706
 WO 1995-AU407 W 19950705

OTHER SOURCE(S): MARPAT 124:234956
 GI

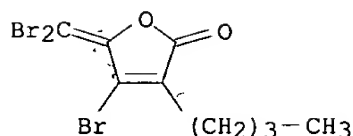


AB An antifouling compn. comprises an effective amt. of a furanone compd. I
 (R1, R2 and R3 = H, OH, C1-10-alkyl, an ether group contg. from 1-10 C
 atoms or R2 and R3 together may comprise an unsubstituted or a
 halogenated
 alkene contg. from 1-10 C atoms; and R4 = a H or halogen atom), and a
 suitable carrier. I (R1 = H, R2-3 = Br) (10 .mu.g/mL in DMSO) inhibited
 settlement of barnacle by 50%, relative to control (without antifoulant).

IT **63025-36-5**
 RL: BUU (Biological use, unclassified); MOA (Modifier or additive use);
 TEM (Technical or engineered material use); BIOL (Biological study); USES
 (Uses)
 (antifouling marine compns. of (substituted) Bu furanone compds.)

RN 63025-36-5 HCAPLUS

CN 2(5H)-Furanone, 4-bromo-3-butyl-5-(dibromomethylene)- (9CI) (CA INDEX
 NAME)



L7 ANSWER 8 OF 24 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1995:789666 HCAPLUS

DOCUMENT NUMBER: 123:281148

TITLE: Broad spectrum effects of secondary metabolites from the red alga *Delisea pulchra* in antifouling assays.

AUTHOR(S): De Nys, R; Steinberg, P D; Willemsen, P; Dworjanyn, S A; Gabelish, C L; King, R J

CORPORATE SOURCE: School of Biological Science, University of New South Wales, Sydney, 2052, Australia

SOURCE: Biofouling (1995), 8(4), 259-71

CODEN: BFOUEC; ISSN: 0892-7014

DOCUMENT TYPE: Journal

LANGUAGE: English

AB In this study the antifouling activity was investigated of a series of chem.-related, halogenated furanones, isolated from *D. pulchra*, a red alga

which is rarely fouled in the field. The metabolites were tested in lab. assays against the barnacle *Balanus amphitrite*, the alga *Ulva lactuca* and a marine bacterium (strain SW 8). Settlement of barnacle cyprid larvae was strongly inhibited, with an $\text{EC}_{50} < 25 \text{ ng} \cdot \text{mL}^{-1}$

(25 ppb) for some compds. The settlement and growth of algal gametes was

also strongly inhibited, in some cases at concns. as low as $25 \text{ ng} \cdot \text{cm}^{-2}$. Growth of the marine bacterium SW8 was inhibited more strongly than by

the common antibiotic gentamicin. Activity of the *D. pulchra* metabolites was comparable to that of the heavy metals and biocides currently used in antifouling paints. However, no single compd. was most active in all tests and some metabolites effective against one organism showed little

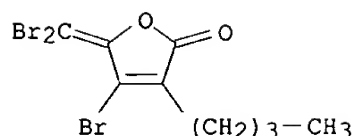
or no activity against the others. The high, but variable level of activity of the *D. pulchra* metabolites, coupled with their small size, relative stability, and ability to be synthesized, suggest their potential use as active ingredients in antifouling coatings.

IT 63025-36-5P

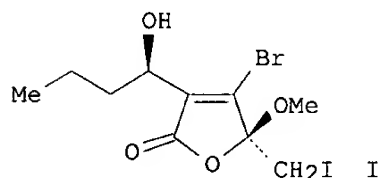
RL: BAC (Biological activity or effector, except adverse); MFM (Metabolic formation); PUR (Purification or recovery); BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation)
(*Delisea pulchra* metabolite as antifouling agent)

RN 63025-36-5 HCAPLUS

CN 2(5H)-Furanone, 4-bromo-3-butyl-5-(dibromomethylene)- (9CI) (CA INDEX NAME)

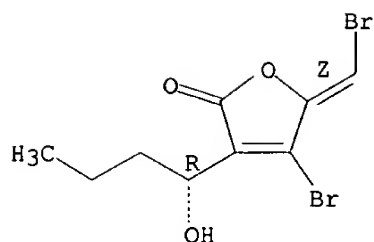


L7 ANSWER 9 OF 24 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1995:609886 HCAPLUS
 DOCUMENT NUMBER: 123:32846
 TITLE: Determination of the absolute configuration of a series of halogenated furanones from the marine alga *Delisea pulchra*
 AUTHOR(S): Koenig, Gabriele M.; Wright, Anthony D.
 CORPORATE SOURCE: Dep. Pharmacy, Swiss Fed. Inst. Technology (ETH), Zurich, CH-8057, Switz.
 SOURCE: Helv. Chim. Acta (1995), 78(3), 758-64
 CODEN: HCACAV; ISSN: 0018-019X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI

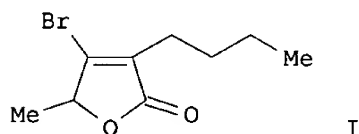


AB The abs. configuration of a series of naturally occurring and semi-synthetic halogenated furanones, e.g., I, is proposed on the basis of chem. interconversions and X-ray and CD analyses. The CD analyses clearly reveal that the presence of the allylic O-atom has a strong influence in detg. the sign and intensity of the low energy $\pi \rightarrow \pi^*$ transition.
 IT 63025-28-5
 RL: RCT (Reactant)
 (abs. configuration of marine alga halogenated furanones)
 RN 63025-28-5 HCAPLUS
 CN 2(5H)-Furanone, 4-bromo-5-(bromomethylene)-3-[(1R)-1-hydroxybutyl]-, (5Z)-
 (9CI) (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry as shown.

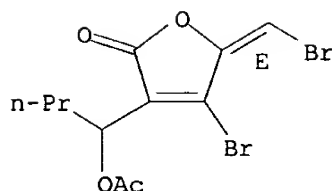


L7 ANSWER 10 OF 24 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1995:433719 HCAPLUS
 DOCUMENT NUMBER: 122:239428
 TITLE: Easy Access to 5-Alkyl-4-bromo-2(5H)-furanones:
 Synthesis of a Fimbroliide, an Acetoxymimbroliide, and
 Bromobeckerelide
 AUTHOR(S): de March, Pedro; Font, Josep; Gracia, Antonio;
 Qingying, Zheng
 CORPORATE SOURCE: Unitat de Química Organica, Universitat Autònoma de
 Barcelona, Bellaterra, 08193, Spain
 SOURCE: J. Org. Chem. (1995), 60(6), 1814-22
 CODEN: JOCEAH; ISSN: 0022-3263
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



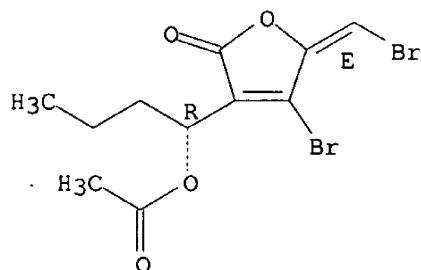
AB Treatment of .gamma.-monosubstituted allenic esters, e.g.,
 MeCH:C:C(CO₂Me)Bu, with N-bromosuccinimide in water yields
 5-alkyl-4-bromo-2(5H)-furanones, e.g., I, that can be transformed into
 5-alkylidene-4-bromo-2(5H)-furanones in good overall yields. Starting
 with a simple allenic ester these transformations have been applied to a
 new synthesis of fimbroliide, acetoxymimbroliide, and bromobeckerelide.
 IT **162426-33-7P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of alkylbromofuranones and access to fimbroliide,
 acetoxymimbroliide, and bromobeckerelide)
 RN 162426-33-7 HCAPLUS
 CN 2(5H)-Furanone, 3-[1-(acetyloxy)butyl]-4-bromo-5-(bromomethylene)-, (E)-
 (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L7 ANSWER 11 OF 24 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1994:49751 HCAPLUS
 DOCUMENT NUMBER: 120:49751
 TITLE: New halogenated furanones from the marine alga
 Delisea pulchra (cf. fimbriata)
 AUTHOR(S): de Nys, Rocky; Wright, Anthony D.; Konig, Gabriele
 M.;
 CORPORATE SOURCE: Sticher, Otto
 Dep. Pharm., Swiss Fed. Inst. Technol., Zurich,
 CH-8057, Switz.
 SOURCE: Tetrahedron (1993), 49(48), 11213-20
 CODEN: TETRAB; ISSN: 0040-4020
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB An investigation of the natural products of the red alga *D. pulchra*,
 collected from the Cape Banks, New South Wales, Australia, yielded eight
 new polyhalogenated furanones and previously reported metabolites. The
 structures of the new compds. were detd. from the interpretation of their
 1D and 2D NMR, UV, IR and mass spectral data. For the first time,
 complete ¹H and ¹³C NMR data for 6 of the previously isolated compds. are
 reported.
 IT 63025-20-7
 RL: BIOL (Biological study)
 (from *Delisea pulchra*)
 RN 63025-20-7 HCAPLUS
 CN 2(5H)-Furanone, 3-[1-(acetyloxy)butyl]-4-bromo-5-(bromomethylene)-,
 [R-(E)]- (9CI) (CA INDEX NAME)

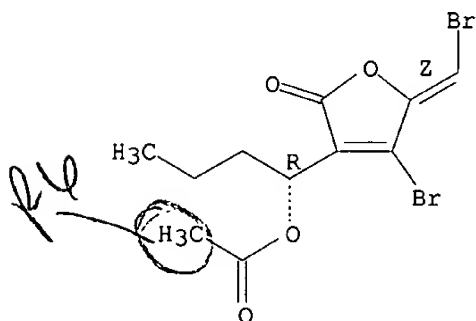
Absolute stereochemistry.
 Double bond geometry as shown.



L7 ANSWER 12 OF 24 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1993:55719 HCAPLUS
 DOCUMENT NUMBER: 118:55719
 TITLE: Delisea pulchra (cf. fimbriata) revisited. The structural determination of two new metabolites from the red alga Delisea pulchra
 AUTHOR(S): De Nys, Rocky; Coll, John C.; Bowden, Bruce F.
 CORPORATE SOURCE: Dep. Chem. Biochem., James Cook Univ., Townsville, 4811, Australia
 SOURCE: Aust. J. Chem. (1992), 45(10), 1625-32
 CODEN: AJCHAS; ISSN: 0004-9425
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Two new metabolites, 1,1,3-tribromododecenol and 6-acetoxy-1,1,2-tribromooctenone, were isolated from D. pulchra. Five previously reported metabolites were also isolated, and the full NMR characterization of 3 fimbrolides is reported for the first time.
 IT 63025-21-8
 RL: BIOL (Biological study)
 (from Delisea pulchra)
 RN 63025-21-8 HCAPLUS
 CN 2(5H)-Furanone, 3-[(1R)-1-(acetyloxy)butyl]-4-bromo-5-(bromomethylene)-, (5Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry as shown.



L7 ANSWER 13 OF 24 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1992:511367 HCAPLUS
 DOCUMENT NUMBER: 117:111367
 TITLE: Bromine addition to .alpha.-(1-hydroxyalkyl)- and .alpha.-(1-alkoxyalkyl)-.alpha.,.beta.-unsaturated esters: an approach to hydroxyfimbrolide and bromobeckerelide
 AUTHOR(S): Calderon, Angel; Font, Josep; De March, Pedro
 CORPORATE SOURCE: Unitat Quim. Org., Univ. Auton. Barcelona, Bellaterra,
 08193, Spain
 SOURCE: Tetrahedron (1992), 48(25), 5347-58
 CODEN: TETRAB; ISSN: 0040-4020
 DOCUMENT TYPE: Journal

LANGUAGE: English

AB Conventional ionic bromination of electron-poor olefins, RO₂CC(:CH₂)CH(OR₁)Pr (R = Me, Et; R₁ = H, Me, CH₂OCH₂CH₂OMe) and Me (E)-2-(1-hydroxyethyl)-2-butenate, proceeds with yields >80%. Treatment of (E)-BrCH:C(CO₂H)CHPrOCH₂OCH₂CH₂OMe with two equiv. of strong bases, a reaction related to a possible hydroxyfimbrolide and bromobeckerlide synthesis, resulted in the halogen-metal exchange reaction affording CH₂:C(CO₂H)CHPrOCH₂OCH₂CH₂OMe, presumably through the generation of a dianion.

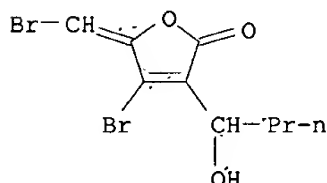
IT **143140-80-1**

RL: RCT (Reactant)

(bromohydroxyalkenoate intermediates for, prepn. of)

RN 143140-80-1 HCAPLUS

CN 2(5H)-Furanone, 4-bromo-5-(bromomethylene)-3-(1-hydroxybutyl)- (9CI) (CA INDEX NAME)



L7 ANSWER 14 OF 24 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1988:489737 HCAPLUS

DOCUMENT NUMBER: 109:89737

TITLE: Novel 2(5H)-furanones from the red marine alga
Delisea

elegans (Lamouroux)

AUTHOR(S): McCombs, John D.; Blunt, John W.; Chambers, Mark V.;
Munro, Murray H. G.; Robinson, Ward T.

CORPORATE SOURCE: Dep. Chem., Univ. Canterbury, Christchurch, N. Z.

SOURCE: Tetrahedron (1988), 44(5), 1489-502

CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 109:89737

AB Six novel 2(5H)-furanones, all related to the previously reported fimbrolide (3-butyl-4-bromo-5-(dibromomethylidene)-2(5H)-furanone), have been isolated from the red marine alga *D. elegans* (family Bonnemaisoniaceae). Three of the six compds., characterized by spectroscopic and single crystal x-ray structure analyses, contain unusual

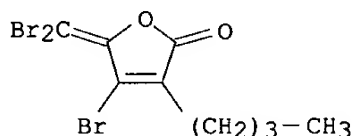
poly-brominated cyclobutane functions.

IT **63025-36-5**

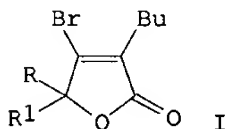
RL: BIOL (Biological study)
(from *Delisea elegans*)

RN 63025-36-5 HCAPLUS

CN 2(5H)-Furanone, 4-bromo-3-butyl-5-(dibromomethylene)- (9CI) (CA INDEX NAME)

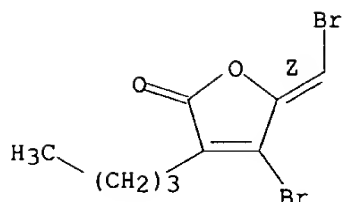


L7 ANSWER 15 OF 24 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1985:406140 HCAPLUS
 DOCUMENT NUMBER: 103:6140
 TITLE: A new synthesis of 3-n-butyl-4-bromo-5(Z)-
 bromomethylidene-2(5H)-furanone, a naturally
 occurring fimbrolide from *Delisia fimbriata* (Bonnemaisoniaceae)
 AUTHOR(S): Caine, Drury; Ukachukwu, Victoria C.
 CORPORATE SOURCE: Sch. Chem., Georgia Inst. Technol., Atlanta, GA,
 30332, USA
 SOURCE: J. Org. Chem. (1985), 50(12), 2195-8
 CODEN: JOCEAH; ISSN: 0022-3263
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 103:6140
 GI



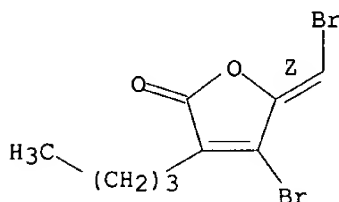
AB The title compd. (I, RR1 = Z-CHBr)(II) was prepd. by addn. of
 BrLiC:CBuCO2Li (III), prepd. by metalation of BrCH:CBuCO2H, to Ac2O to
 give I (R = Me, R1 = OH). Dehydration of the latter compd. with P2O5
 gave I (RR1 = CH2), which was brominated with Br followed by
 dehydrobromination with DBU to give II in 41% overall yield. Addn. of III to Cl3CCHO gave I
 (R = CCl3, R1 = H) which was dehydrochlorinated with DBU to give I (RR1 =
 CCl2) in 55% overall yield.
 IT **63025-35-4P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 RN 63025-35-4 HCAPLUS
 CN 2(5H)-Furanone, 4-bromo-5-(bromomethylene)-3-butyl-, (5Z)- (9CI) (CA
 INDEX NAME)

Double bond geometry as shown.



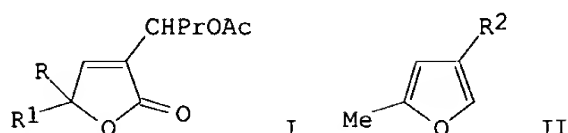
L7 ANSWER 16 OF 24 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1983:600391 HCAPLUS
 DOCUMENT NUMBER: 99:200391
 TITLE: Antimicrobial constituents [of marine algae]
 AUTHOR(S): Ochi, Masamitsu
 CORPORATE SOURCE: Fac. Sci., Kochi Univ., Kochi, Japan
 SOURCE: Suisangaku Shiriizu (1983), 45(Kaiso no
 Seikagaku to Riyo), 101-19
 CODEN: SUSHDC
 DOCUMENT TYPE: Journal
 LANGUAGE: Japanese
 AB Antimicrobial substances were isolated from a wide variety (131 strains)
 of seaweeds growing along the coast of Japan. The antimicrobial
 activities of the compds. against Staphylococcus aureus, Bacillus
 subtilis, Escherichia coli, Saccharomyces cerevisiae, etc. were shown.
 IT 63025-35-4
 RL: BAC (Biological activity or effector, except adverse); BIOL
 (Biological study)
 (of seaweed, antimicrobial activity of)
 RN 63025-35-4 HCAPLUS
 CN 2(5H)-Furanone, 4-bromo-5-(bromomethylene)-3-butyl-, (5Z)- (9CI) (CA
 INDEX NAME)

Double bond geometry as shown.



L7 ANSWER 17 OF 24 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1983:539591 HCAPLUS
 DOCUMENT NUMBER: 99:139591
 TITLE: Efficient synthesis of acetoxymimbrolides and
 beckerelide analogs
 AUTHOR(S): Kotsuki, Hiyoshizo; Monden, Mitsugu; Ochi, Masamitsu
 CORPORATE SOURCE: Fac. Sci., Kochi Univ., Kochi, 780, Japan
 SOURCE: Chem. Lett. (1983), (7), 1007-8
 CODEN: CMLTAG; ISSN: 0366-7022

DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB The title compds. I (RR1 = CH₂, CHBr) were prepd. from II (R₂ = CHO) by Grignard reaction with PrI, 3-ClC₆H₄CO₂OH oxidn. of II (R₂ = CHPrOAc), dehydration of I (R = Me, R₁ = OH) with P₂O₅, and bromination. I (RR₁ = CH₂, CHBr) had a min. inhibitory concn. against *Aspergillus niger* of 50 and 25 .mu.g/mL resp., whereas I (R = Me, R₁ = OH) was inactive.

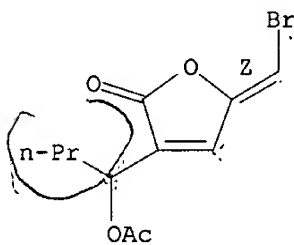
IT **87241-09-6P**

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (prepn. and fungicidal activity of)

RN 87241-09-6 HCAPLUS

CN 2(5H)-Furanone, 3-[1-(acetyloxy)butyl]-5-(bromomethylene)-, (Z)- (9CI)
 (CA INDEX NAME)

Double bond geometry as shown.



L7 ANSWER 18 OF 24 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1980:508527 HCAPLUS

DOCUMENT NUMBER: 93:108527

TITLE: Marine natural products affecting neurotransmission

AUTHOR(S): Taylor, K. M.; Spence, I.

CORPORATE SOURCE: Roche Res. Inst. Mar. Pharmacol., Dee Why, 2099, Australia

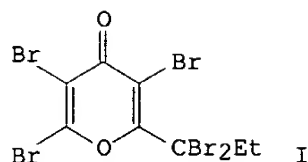
SOURCE: Neurotoxins: Fundam. Clin. Adv., [Int. Conf.] (1979), 85-93. Editor(s): Chubb, I. W.; Geffen, L. B. Adelaide Univ. Union Press: Adelaide, Australia.

CODEN: 43IFAS

DOCUMENT TYPE: Conference

LANGUAGE: English

GI



AB Conus geographus Crude venom caused a reversible block of muscle excitability and decreased neuromuscular transmission in the phrenic nerve-diaphragm prepn.; these activities were due to 3 polypeptide present in the crude venom. Marine substances, e.g. furanoquinol [65557-84-8], pentabromopropylpyrone (I) [69267-70-5], acetoxymimbrolide [74365-48-3], and aminooxyacetic acid [471-47-6], were potent inhibitors of GABA [56-12-2] neurochem. processes, but their specificity was limited, esp. by their inhibitory effects on mitochondrial respiration. Polyhalogenated monoterpenes isolated from red algae had central nervous system depressant activity in animals. The exception was Plocamadiene A [66321-25-3] isolated from Plocamium cartilagineum which caused a reversible spastic paresis in mice. The severe muscle spasm was antagonized by diazepam [439-14-5].

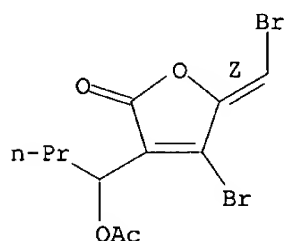
IT 74365-48-3

RL: ADV (Adverse effect, including toxicity); BIOL (Biological study) (neurochem. activity and toxicity of)

RN 74365-48-3 HCAPLUS

CN 2(5H)-Furanone, 3-[1-(acetyloxy)butyl]-4-bromo-5-(bromomethylene)-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L7 ANSWER 19 OF 24 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1980:431673 HCAPLUS

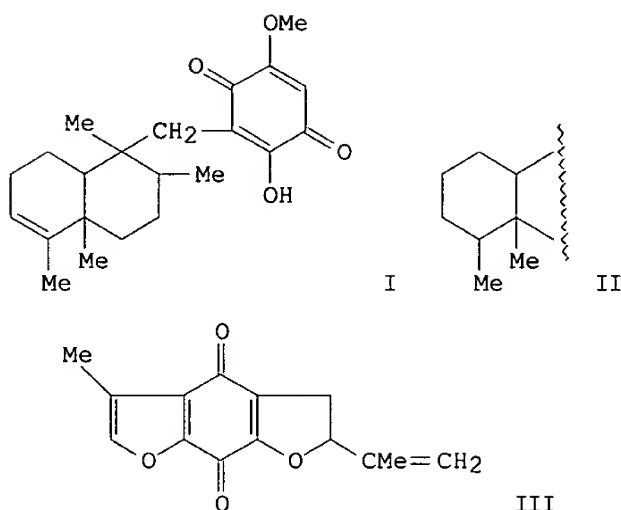
DOCUMENT NUMBER: 93:31673

TITLE: Potent inhibition of oxidative phosphorylation by marine natural products

AUTHOR(S): Jamieson, Dana D.; De Rome, Paul J.; Taylor, Kenneth M.

CORPORATE SOURCE: Roche Res. Inst. Mar. Pharmacol., Dee Why, 2099, Australia

SOURCE: J. Pharm. Sci. (1980), 69(4), 462-5
 CODEN: JPMSAE; ISSN: 0022-3549
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB Many lipid-sol. exts. from various marine organisms have a nonspecific depressant effect on smooth muscle contractions. Novel compds. isolated from such lipid-sol. exts. were tested for their effects on the respiration of rat liver mitochondria and produced potent stimulation or inhibition of oxygen uptake by the mitochondria. Isospongiaquinone (I) [69672-66-8] and dihydroisospongiaquinone (II) [69672-74-8], extd. from sponge, produced .apprx.50% inhibition of State 3 respiration at 1 .mu.M; at 5.mu.M considerable depression of State 4 respiration was seen. The most potent stimulant of State 4 respiration was dihydrocyparaquinone (III) [27304-02-5], which approx. doubled State 4 respiration at 4 .mu.M.

Other compds. such as costatol [63023-57-4], heterocladol [65746-13-6], and acetoxymbrolide [63025-21-8] showed mixed stimulation of State 4 and inhibition of State 3 respiration.

IT 63025-21-8

RL: BIOL (Biological study)

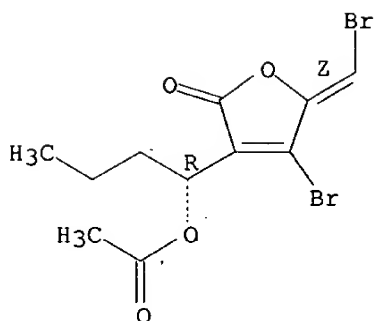
(of red algae, oxidative phosphorylation in relation to)

RN 63025-21-8 HCAPLUS

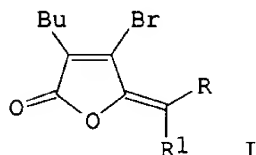
CN 2(5H)-Furanone, 3-[(1R)-1-(acetyloxy)butyl]-4-bromo-5-(bromomethylene)-, (5Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

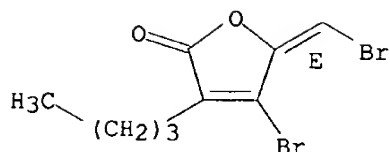
Double bond geometry as shown.



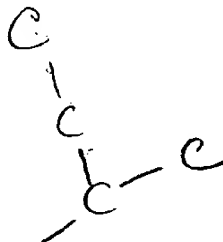
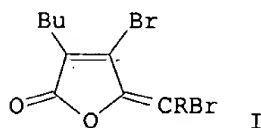
L7 ANSWER 20 OF 24 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1979:592772 HCAPLUS
 DOCUMENT NUMBER: 91:192772
 TITLE: The first synthesis of fimbrolides, a novel class of halogenated lactones naturally occurring in the red seaweed *Delisea fimbriata* (Bonnemaisoniaceae)
 AUTHOR(S): Beechan, Curtis M.; Sims, James J.
 CORPORATE SOURCE: Dep. Plant Pathol., Univ. California, Riverside, CA, USA
 SOURCE: Tetrahedron Lett. (1979), (19), 1649-52
 CODEN: TELEAY; ISSN: 0040-4039
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB BuCHBrCO₂Et on sequential condensation reaction with MeCOCH₂CO₂Et, hydrolysis, thermal decarboxylation and bromination gave HO₂CCHBuCHBrCOCH₂Br, which on treatment with 100% H₂SO₄ at 100.degree. underwent intramol. cyclocondensation reaction to give fimbrolide I (R = H, R₁ = Br) together with a very small amt. of I (R = Br, R₁ = H).
 IT **63025-34-3P**
 RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)
 RN 63025-34-3 HCAPLUS
 CN 2(5H)-Furanone, 4-bromo-5-(bromomethylene)-3-butyl-, (E)- (9CI) (CA INDEX NAME)
 Double bond geometry as shown.



L7 ANSWER 21 OF 24 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1978:135794 HCAPLUS
 DOCUMENT NUMBER: 88:135794
 TITLE: Identification of halogen substituents in natural products by measurement of carbon-13 spin-lattice relaxation times and integrated intensities
 AUTHOR(S): Norton, Raymond S.
 CORPORATE SOURCE: Roche Res. Inst. Mar. Pharmacol., Dee Why, Aust.
 SOURCE: Tetrahedron (1977), 33(19), 2577-81
 CODEN: TETRAB; ISSN: 0040-4020
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



103

AB A method is proposed for differentiating brominated from chlorinated C atoms by natural-abundance ^{13}C NMR spectroscopy. Spin-lattice relaxation behavior of brominated C atoms is influenced by C-Br scalar interactions, which lead to shortened ^{13}C spin-lattice relaxation times and reduced values of nuclear Overhauser enhancement. C-Cl scalar interactions make

a negligible contribution to the spin-lattice relaxation of chlorinated C. These effects were illustrated by measuring the ^{13}C spin-lattice relaxation times and integrated intensities of PhR (R = Cl, Br, iodo), chloro-, bromo- and iodocyclohexane, costatol, costatone and the fimbrolides I (R = Br, H). ^{13}C relaxation measurements can be used to distinguish brominated from chlorinated C in the case of halogenated quaternary C atoms, sp^2 -hybridized methine C, and some sp^3 -hybridized methine C.

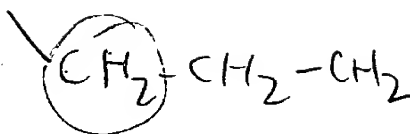
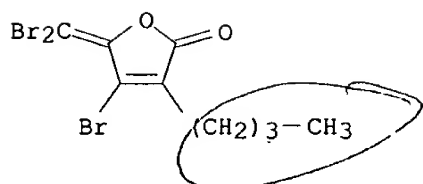
IT 63025-36-5

RL: PRP (Properties)

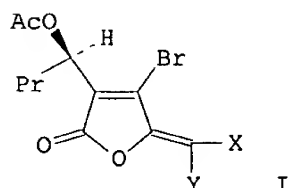
(carbon-13 spin-lattice relaxation and integrated intensities of)

RN 63025-36-5 HCAPLUS

CN 2(5H)-Furanone, 4-bromo-3-butyl-5-(dibromomethylene)- (9CI) (CA INDEX NAME)



L7 ANSWER 22 OF 24 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1978:3069 HCAPLUS
DOCUMENT NUMBER: 88:3069
TITLE: Natural products from the red seaweed *Delisea fimbriata*
AUTHOR(S): Sims, J. J.; Pettus, J. A., Jr.; Wing, R. M.
CORPORATE SOURCE: Dep. Chem., Univ. California, Riverside, Calif., USA
SOURCE: NATO Conf. Ser., [Ser.] 4 (1977), 1(Mar.
Nat. Prod. Chem.), 205-9
CODEN: NCSFDT
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



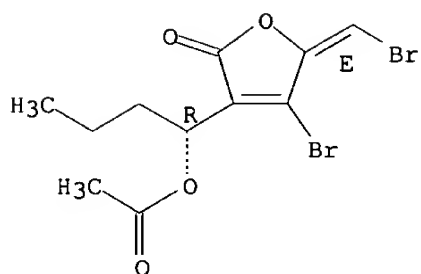
AB The red seaweed *D. fimbriata*, on extn. with CH₂Cl₂ and MeOH, yielded 2 fractions, a lactonic fraction and a less polar fraction. The lactone fraction on high pressure liq. chromatog. gave 7 compds. identified by spectral and chem. anal. as I, where X = H, Br, or I and Y = H, Br, Cl,

I. The less polar fraction was sepd. by chromatog. into 5 halogenated ketones ($\text{BuCHXCOCY} \cdot \text{CBr}_2$, where $\text{X} = \text{H, Br, or Cl}$ and $\text{Y} = \text{Br or I}$). The ketones were identified by synthesis and from spectral data.

RL: BOC (Biological occurrence); BIOL (Biological study); OCCU
(Occurrence)
(of seaweed)

2(5H)-Furanone, 3-[1-(acetyloxy)butyl]-4-bromo-5-(bromomethylene)-,
[R(E)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L7 ANSWER 23 OF 24 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1977:189143 HCAPLUS

DOCUMENT NUMBER: 86:189143

TITLE: Marine natural products. XII. Isolation of a family of multihalogenated gamma-methylene lactones from the red seaweed *Delisea fimbriata*

AUTHOR(S): Pettus, John A., Jr.; Wing, Richard M.; Sims, James J.

CORPORATE SOURCE: Dep. Chem., Univ. California, Riverside, Calif., USA

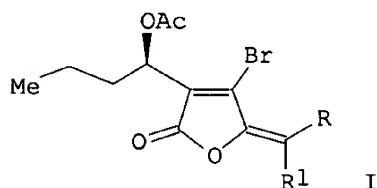
SOURCE: Tetrahedron Lett. (1977), (1), 41-4

CODEN: TELEAY

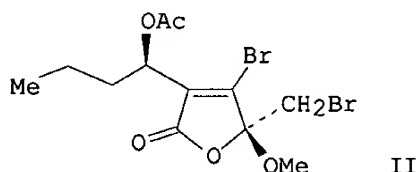
DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I



II

AB The mol. structures of the acetoxyfimbrolides I (R = H, R1 = Br, I, Cl; R = Br, R1 = H, Br; R = I, R1 = H), isolated from the thallus of *D. fimbriata*, were detd. from spectral data. I (R = H, R1 = Br) with MeOH gave II, the crystal structure of which was detd. by x-ray anal.

IT 63025-20-7P

RL: PREP (Preparation)

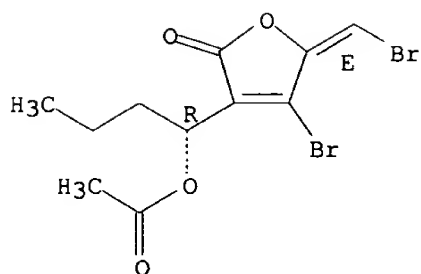
(from *Delisea fimbriata*, mol. structure of)

RN 63025-20-7 HCAPLUS

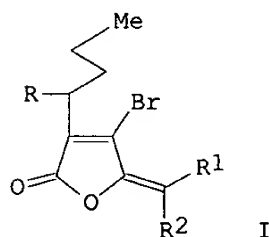
CN 2(5H)-Furanone, 3-[1-(acetyloxy)butyl]-4-bromo-5-(bromomethylene)-, [R-(E)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

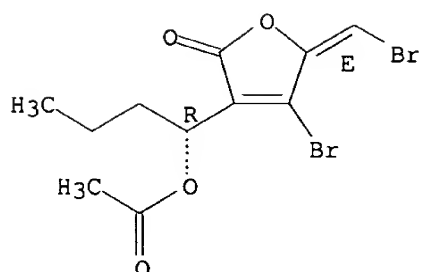


L7 ANSWER 24 OF 24 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1977:189142 HCAPLUS
 DOCUMENT NUMBER: 86:189142
 TITLE: A new class of halogenated lactones from the red alga
 Delisea fimbriata (Bonnemaisioniaceae)
 AUTHOR(S): Kazlauskas, R.; Murphy, P. T.; Quinn, R. J.; Wells,
 R.
 J.
 CORPORATE SOURCE: Roche Res. Inst. Mar. Pharmacol., Dee Why, Aust.
 SOURCE: Tetrahedron Lett. (1977), (1), 37-40
 CODEN: TELEAY
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB The mol. structures of the fimbrolides I (R = OAc, OH, R1 = H, R2 = Br,
 I,
 Cl; R = OAc, OH, R1 = Br, I, Cl, R2 = H; R = OAc, OH, R1 = R2 = Br; R =
 R2
 = H, R1 = Br; R = R1 = H, R2 = Br; R = H, R1 = R2 = Br), isolated from D.
 fimbriata, were detd. from chem. and spectral data.
 IT 63025-20-7P
 RL: PREP (Preparation)
 (from Delisea fimbriata, mol. structure of)
 RN 63025-20-7 HCAPLUS
 CN 2(5H)-Furanone, 3-[1-(acetyloxy)butyl]-4-bromo-5-(bromomethylene)-,
 [R-(E)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry as shown.



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L2 1 S L1

L3 79 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 03:49:50 ON 01 JUL 2002

L4 43 S L3

L5 25 S L4 AND PD < MAY 1998
 L6 5 S L4 AND READ, R?/AU
 L7 24 S L5 NOT L6

FILE 'CAOLD' ENTERED AT 03:51:30 ON 01 JUL 2002

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L8 0 L3

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